Supplementary Material (ESI) for CrystEngComm

0D, 2D and 3D metal phosphonates assembled from a new 2'-carboxybiphenyl-4-ylmethylphosphonic acid: syntheses, topological structures and photoluminescent properties

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Table S1a. Selected bond distances (Å) and angles (°) for **L**.

P(1)-O(3)	1.503(2)	P(1)-O(1)	1.531(2)
P(1)-O(2)	1.550(2)	O(3)-P(1)-O(1)	113.93(11)
O(3)-P(1)-O(2)	112.98(10)	O(1)-P(1)-O(2)	102.68(12)

Table S1b. Hydrogen bonds for **L** (Å and °).

D-H···A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2)...O(3)#1	0.82	1.83	2.604(3)	156.1
O(1)-H(1)...O(3)#2	0.82	1.90	2.617(3)	145.0
O(5)-H(5)...O(4)#3	0.82	1.83	2.635(3)	167.0

Symmetry codes for **L**: [#1] -x, -y - 1, -z + 1 ; [#2] -x, -y, -z + 1 ; [#3] –x + 1, -y + 1, -z.

Table S2a. Selected bond distances (Å) and angles (°) for **1**.

Cu(1)-O(3)#1	1.929(3)	Cu(1)-O(2)#2	1.937(4)
Cu(1)-O(1W)	1.942(3)	Cu(1)-O(1)	1.969(3)
Cu(1)-O(1W')	2.007(14)	O(3)#1-Cu(1)-O(2)#2	96.58(13)
O(3)#1-Cu(1)-O(1W)	91.31(18)	O(2)#2-Cu(1)-O(1W)	171.00(18)
O(3)#1-Cu(1)-O(1)	171.50(15)	O(2)#2-Cu(1)-O(1)	86.37(12)
O(1W)-Cu(1)-O(1)	86.42(16)	O(3)#1-Cu(1)-O(1W')	88.3(5)
O(2)#2-Cu(1)-O(1W')	151.2(6)	O(1W)-Cu(1)-O(1W')	32.9(5)
O(1)-Cu(1)-O(1W')	85.3(5)		

Table S2b. Hydrogen bonds for **1** (Å and °).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(4)-H(4A)...O(1)#1	0.82	1.86	2.676(5)	177.4

Symmetry codes for **1**: [#1] –x + 2, y + 1/2, -z + 1 ; [#2] –x + 3, y + 1/2, -z + 1.

Table S3. Selected bond distances (Å) and angles (°) for **2**.

Cu(1)-O(6)	1.882(5)	Cu(1)-O(1)#1	1.950(5)
Cu(1)-O(4)	1.953(5)	Cu(1)-O(7)#2	1.998(4)
Cu(1)-O(3)#3	2.393(5)	Cu(3)-O(3)#4	1.906(5)
Cu(3)-O(7)	1.987(5)	Cu(2)-O(6)	1.888(4)
Cu(2)-O(2)#4	1.932(5)	Cu(2)-O(7)	1.963(4)
Cu(2)-O(5)	1.969(6)	O(6)-Cu(1)-O(1)#1	96.0(2)

O(6)-Cu(1)-O(4)	95.3(2)	O(1)#1-Cu(1)-O(4)	161.6(2)
O(6)-Cu(1)-O(7)#2	176.3(2)	O(1)#1-Cu(1)-O(7)#2	83.98(19)
O(4)-Cu(1)-O(7)#2	85.6(2)	O(6)-Cu(1)-O(3)#3	103.7(2)
O(1)#1-Cu(1)-O(3)#3	101.5(2)	O(4)-Cu(1)-O(3)#3	89.8(2)
O(7)#2-Cu(1)-O(3)#3	72.67(17)	O(3)#4-Cu(3)-O(7)#6	95.39(19)
O(3)#5-Cu(3)-O(7)#6	84.61(19)	O(6)-Cu(2)-O(2)#4	91.9(2)
O(6)-Cu(2)-O(7)	167.9(2)	O(2)#5-Cu(2)-O(7)	93.65(19)
O(6)-Cu(2)-O(5)	95.8(2)	O(2)#5-Cu(2)-O(5)	149.4(3)
O(7)-Cu(2)-O(5)	84.8(2)		

Symmetry codes for **2**: [#1] –x + 1, y - 1/2, -z + 3/2 ; [#2] x, -y + 1/2, z - 1/2 ; [#3] –x + 1, -y + 1, -z + 2 ; #[4] –x + 1, y - 1/2, -z + 5/2 ; [#6] –x + 1, -y, -z + 3.

Table S4. Selected bond distances (Å) and angles (°) for **3**.

Zn(1)-O(3)#1	1.866(3)	Zn(1)-O(9)	1.949(3)
Zn(1)-O(5)	1.968(3)	Zn(1)-O(6)#2	1.969(3)
Zn(2)-O(1)#3	1.879(3)	Zn(2)-O(10)	1.950(3)
Zn(2)-O(1W)	1.972(3)	Zn(2)-O(6)#2	2.014(3)
Zn(3)-O(8)#4	1.905(3)	Zn(3)-O(2)#1	1.911(3)
Zn(3)-O(4)	1.941(3)	Zn(3)-O(7)#2	1.968(3)
O(3)#1-Zn(1)-O(9)	119.26(14)	O(3)#1-Zn(1)-O(5)	112.22(15)
O(9)-Zn(1)-O(5)	96.20(15)	O(3)#1-Zn(1)-O(6)#2	117.12(15)
O(9)-Zn(1)-O(6)#2	100.01(14)	O(5)-Zn(1)-O(6)#2	109.58(14)
O(1)#3-Zn(2)-O(10)	117.81(14)	O(1)#3-Zn(2)-O(1W)	103.73(14)
O(10)-Zn(2)-O(1W)	99.72(15)	O(1)#3-Zn(2)-O(6)#2	110.50(14)
O(10)-Zn(2)-O(6)#2	100.21(14)	O(1W)-Zn(2)-O(6)#2	125.41(13)
O(8)#4-Zn(3)-O(2)#1	108.08(15)	O(8)#4-Zn(3)-O(4)	108.00(14)
O(2)#1-Zn(3)-O(4)	114.76(15)	O(8)#4-Zn(3)-O(7)#2	105.94(14)
O(2)#1-Zn(3)-O(7)#2	114.58(14)	O(4)-Zn(3)-O(7)#2	104.97(15)

Symmetry codes for **3**: [#1] x, -y - 1/2, z + 1/2 ; [#2] –x + 1, y - 1/2, -z + 3/2 ; [#3] –x + 1, y + 1/2, -z + 3/2 ; [#4] x, y - 1, z.

Table S5. Selected bond distances (Å) and angles (°) for **4**

Zn(1)-O(1)	1.976(2)	Zn(1)-O(8)#1	2.042(2)

Zn(1)-O(2W)	2.053(2)	Zn(1)-N(3)	2.167(3)
Zn(1)-N(4)	2.191(3)	Zn(2)-O(6)	1.872(3)
Zn(2)-O(3)	1.889(2)	Zn(2)-O(7)#1	1.932(2)
Zn(2)-O(10)#2	1.993(3)	Zn(3)-O(2)#3	1.942(3)
Zn(3)-O(5)	1.963(3)	Zn(3)-N(2)	2.119(3)
Zn(3)-N(1)	2.163(3)	Zn(3)-O(1W)	2.231(3)
O(1)-Zn(1)-O(8)#1	93.86(10)	O(1)-Zn(1)-O(2W)	110.61(11)
O(8)#1-Zn(1)-O(2W)	111.44(10)	O(1)-Zn(1)-N(3)	162.12(11)
O(8)#1-Zn(1)-N(3)	90.07(10)	O(2W)-Zn(1)-N(3)	83.95(11)
O(1)-Zn(1)-N(4)	91.27(11)	O(8)#1-Zn(1)-N(4)	144.26(12)
O(2W)-Zn(1)-N(4)	99.61(11)	N(3)-Zn(1)-N(4)	75.64(11)
O(6)-Zn(2)-O(3)	113.24(14)	O(6)-Zn(2)-O(7)#1	105.18(12)
O(3)-Zn(2)-O(7)#1	117.75(11)	O(6)-Zn(2)-O(10)#2	113.24(14)
O(3)-Zn(2)-O(10)#2	97.75(12)	O(7)#1-Zn(2)-O(10)#2	109.93(11)
O(2)#3-Zn(3)-O(5)	108.65(12)	O(2)#3-Zn(3)-N(2)	127.53(12)
O(5)-Zn(3)-N(2)	123.81(11)	O(2)#3-Zn(3)-N(1)	89.18(12)
O(5)-Zn(3)-N(1)	104.47(12)	N(2)-Zn(3)-N(1)	77.82(12)
O(2)#3-Zn(3)-O(1W)	95.80(10)	O(5)-Zn(3)-O(1W)	88.06(11)
N(2)-Zn(3)-O(1W)	87.40(11)	N(1)-Zn(3)-O(1W)	164.31(11)

Symmetry codes for **4**: $^{\#1}$ x - 1/2, -y + 1/2, -z + 1 ; $^{\#2}$ x + 1/2, -y + 1/2, -z + 1 ; $^{\#3}$ –x + 3, y - 1/2, -z + 3/2.

Table S6a. Selected bond distances (Å) and angles (°) for **5.**

Cd(2)-O(2)#1	2.205(2)	Cd(2)-O(4)	2.295(3)
Cd(2)-O(1)#2	2.300(3)	Cd(2)-O(2)#3	2.335(3)
Cd(2)-O(3)#2	2.396(3)	Cd(2)-O(5)	2.473(2)
Cd(2)-C(14)	2.735(4)	Cd(1)-O(1)	2.282(2)
Cd(1)-O(1W)	2.301(3)	Cd(1)-O(3)#1	2.329(2)
O(2)#1-Cd(2)-O(4)	133.53(9)	O(2)#1-Cd(2)-O(1)#2	136.58(9)
O(4)-Cd(2)-O(1)#2	88.42(9)	O(2)#1-Cd(2)-O(2)#3	75.68(9)
O(4)-Cd(2)-O(2)#3	90.26(9)	O(1)#2-Cd(2)-O(2)#3	97.16(8)

O(2)#1-Cd(2)-O(3)#2	93.20(8)	O(4)-Cd(2)-O(3)#2	123.68(8)
O(1)#2-Cd(2)-O(3)#2	63.26(8)	O(2)#3-Cd(2)-O(3)#2	137.73(9)
O(2)#1-Cd(2)-O(5)	108.85(8)	O(4)-Cd(2)-O(5)	53.90(9)
O(1)#2-Cd(2)-O(5)	105.58(8)	O(2)#3-Cd(2)-O(5)	135.84(8)
O(3)#2-Cd(2)-O(5)	86.43(8)		

Table S6b. Hydrogen bonds for **5** (Å and °).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1W)-H(1)...O(5)#6	0.85	1.84	2.667(2)	164.7
O(1W)-H(1')...O(4)#2	0.85	1.98	2.814(4)	167.3

Symmetry codes for **5**: [#1] x - 1/2, -y - 1/2, -z ; [#2] –x + 1, -y, -z ; [#3] –x + 3/2, y + 1/2, z ; [#4] –x + 1, -y - 1, -z ; [#5] –x + 3/2, y - 1/2, z ; [#6] x + 1/2, -y - 1/2, -z.

Table S7. Selected bond distances (Å) and angles (°) for **6.**

Cd(1)-O(1)	2.201(4)	Cd(1)-O(4)#1	2.245(5)
Cd(1)-O(2)#2	2.279(4)	Cd(1)-O(6)#3	2.282(4)
Cd(1)-O(3)#3	2.299(4)	Cd(1)-O(5)#1	2.539(12)
Cd(2)-O(2W)	2.088(10)	Cd(2)-O(6)	2.231(4)
Cd(2)-O(3)#4	2.245(4)	Cd(2)-O(6)#5	2.295(4)
Cd(2)-O(2)	2.312(4)	Cd(2)-O(1W)	2.354(9)
Cd(2)-O(2W')	2.471(9)	O(1)-Cd(1)-O(4)#1	155.93(18)
O(1)-Cd(1)-O(2)#2	90.62(15)	O(4)#1-Cd(1)-O(2)#2	96.98(17)
O(1)-Cd(1)-O(6)#3	84.51(14)	O(4)#1-Cd(1)-O(6)#3	92.02(18)
O(2)#2-Cd(1)-O(6)#3	167.60(14)	O(1)-Cd(1)-O(3)#3	105.55(15)
O(4)#1-Cd(1)-O(3)#3	98.5(2)	O(2)#2-Cd(1)-O(3)#3	75.33(14)
O(6)#3-Cd(1)-O(3)#3	94.96(14)	O(1)-Cd(1)-O(5)#1	107.4(3)
O(4)#1-Cd(1)-O(5)#1	48.5(3)	O(2)#2-Cd(1)-O(5)#1	105.3(3)
O(6)#3-Cd(1)-O(5)#1	87.1(3)	O(3)#3-Cd(1)-O(5)#1	147.0(3)
O(2W)-Cd(2)-O(6)	134.7(4)	O(2W)-Cd(2)-O(3)#4	113.2(4)
O(6)-Cd(2)-O(3)#4	112.04(16)	O(2W)-Cd(2)-O(6)#5	88.1(3)

O(6)-Cd(2)-O(6)#5	80.24(15)	O(3)#4-Cd(2)-O(6)#5	108.30(14)
O(2W)-Cd(2)-O(2)	92.2(3)	O(6)-Cd(2)-O(2)	96.35(14)
O(3)#4-Cd(2)-O(2)	75.71(14)	O(6)#5-Cd(2)-O(2)	175.45(13)
O(2W)-Cd(2)-O(1W)	46.6(4)	O(6)-Cd(2)-O(1W)	89.3(2)
O(3)#4-Cd(2)-O(1W)	154.1(2)	O(6)#5-Cd(2)-O(1W)	89.1(3)
O(2)-Cd(2)-O(1W)	87.9(3)	O(2W)-Cd(2)-O(2W')	29.1(4)
O(6)-Cd(2)-O(2W')	163.4(3)	O(3)#4-Cd(2)-O(2W')	84.5(3)
O(6)#5-Cd(2)-O(2W')	92.8(2)	O(2)-Cd(2)-O(2W')	89.7(2)
O(1W)-Cd(2)-O(2W')	75.4(3)		

Symmetry codes for **6**: [#1] –x + 1, -y, -z + 1 ; [#2] –x + 1, -y, -z + 2 ; [#3] –x + 1, y - 1/2, -z + 3/2 ; [#4] x, -y + 1/2, z + 1/2 ; [#5] –x + 1, -y +1, -z + 2.

Table S8a. Selected bond distances (Å) and angles (°) for **7.**

Cd(1)-O(2)#1	2.173(2)	Cd(1)-O(4)	2.324(3)
Cd(1)-N(4)	2.342(4)	Cd(1)-N(1)	2.384(4)
Cd(1)-N(2)	2.396(4)	Cd(1)-N(3)	2.455(3)
O(2)#1-Cd(1)-O(4)	103.35(11)	O(2)#1-Cd(1)-N(4)	98.24(11)
O(4)-Cd(1)-N(4)	85.08(13)	O(2)#1-Cd(1)-N(1)	164.03(12)
O(4)-Cd(1)-N(1)	83.80(13)	N(4)-Cd(1)-N(1)	96.58(13)
O(2)#1-Cd(1)-N(2)	94.24(10)	O(4)-Cd(1)-N(2)	116.80(13)
N(4)-Cd(1)-N(2)	151.50(12)	N(1)-Cd(1)-N(2)	69.82(12)
O(2)#1-Cd(1)-N(3)	91.18(10)	O(4)-Cd(1)-N(3)	152.82(13)
N(4)-Cd(1)-N(3)	70.01(12)	N(1)-Cd(1)-N(3)	88.30(13)
N(2)-Cd(1)-N(3)	84.26(12)		

Table S8b. Hydrogen bonds for **7** (Å and °).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3')...O(5)#1	0.86	1.73	2.575(4)	165.9

Symmetry codes for **7**: [#1] –x + 1, -y + 1, -z + 2.

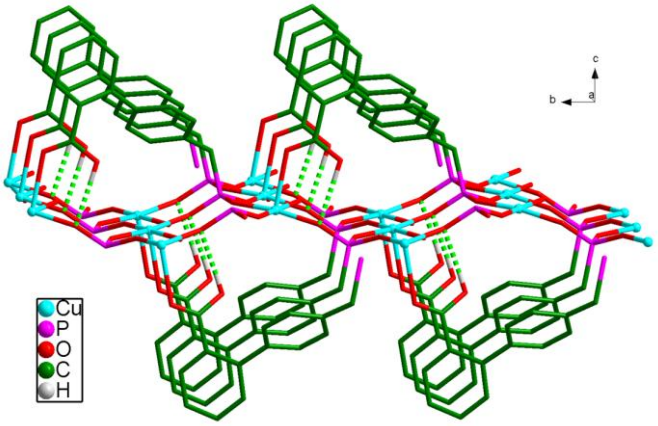

Fig. S1 Hydrogen bonds in complex **1.**

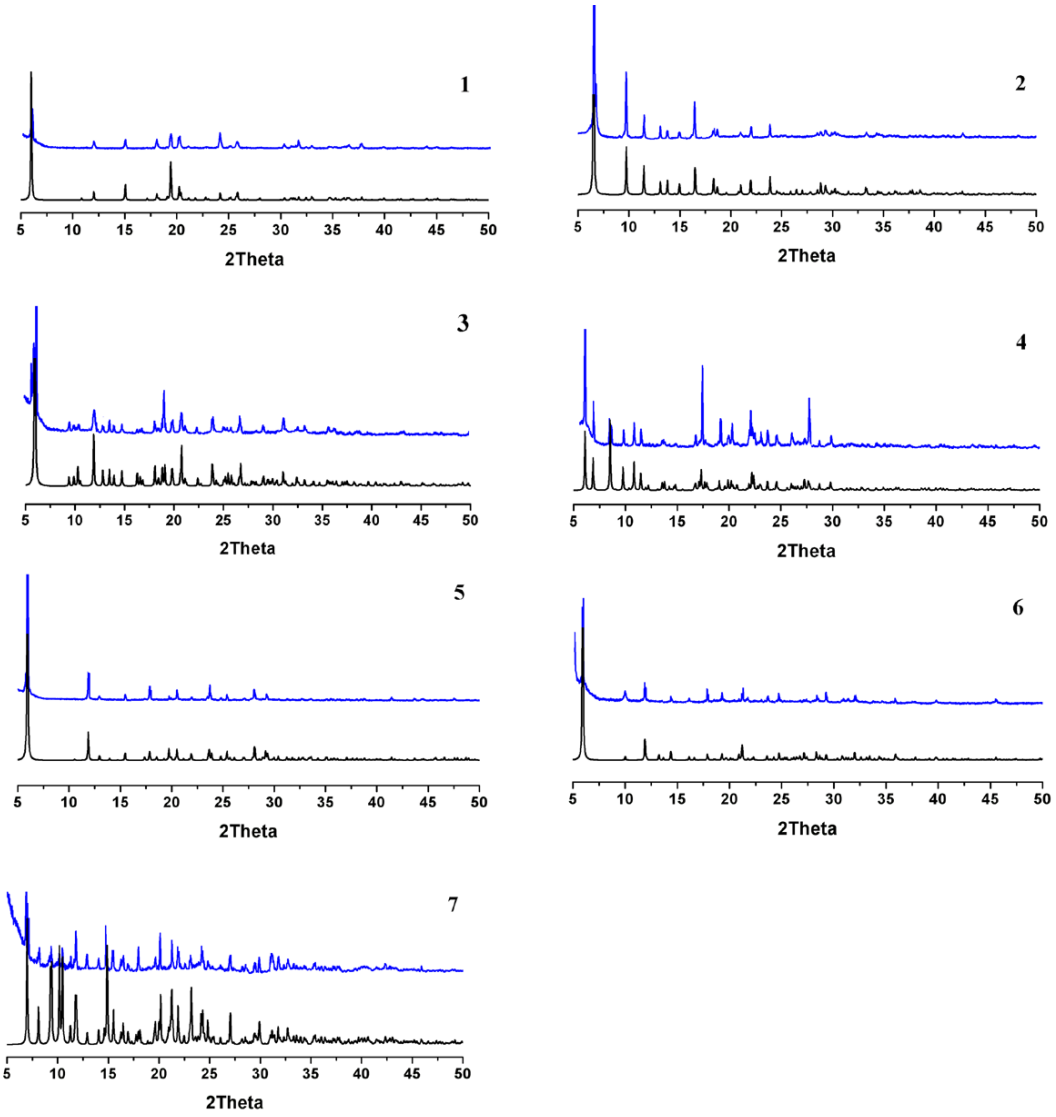

Fig. S2 The simulated (black) and experimental (blue) PXRD patterns for compounds **1**-**7**.

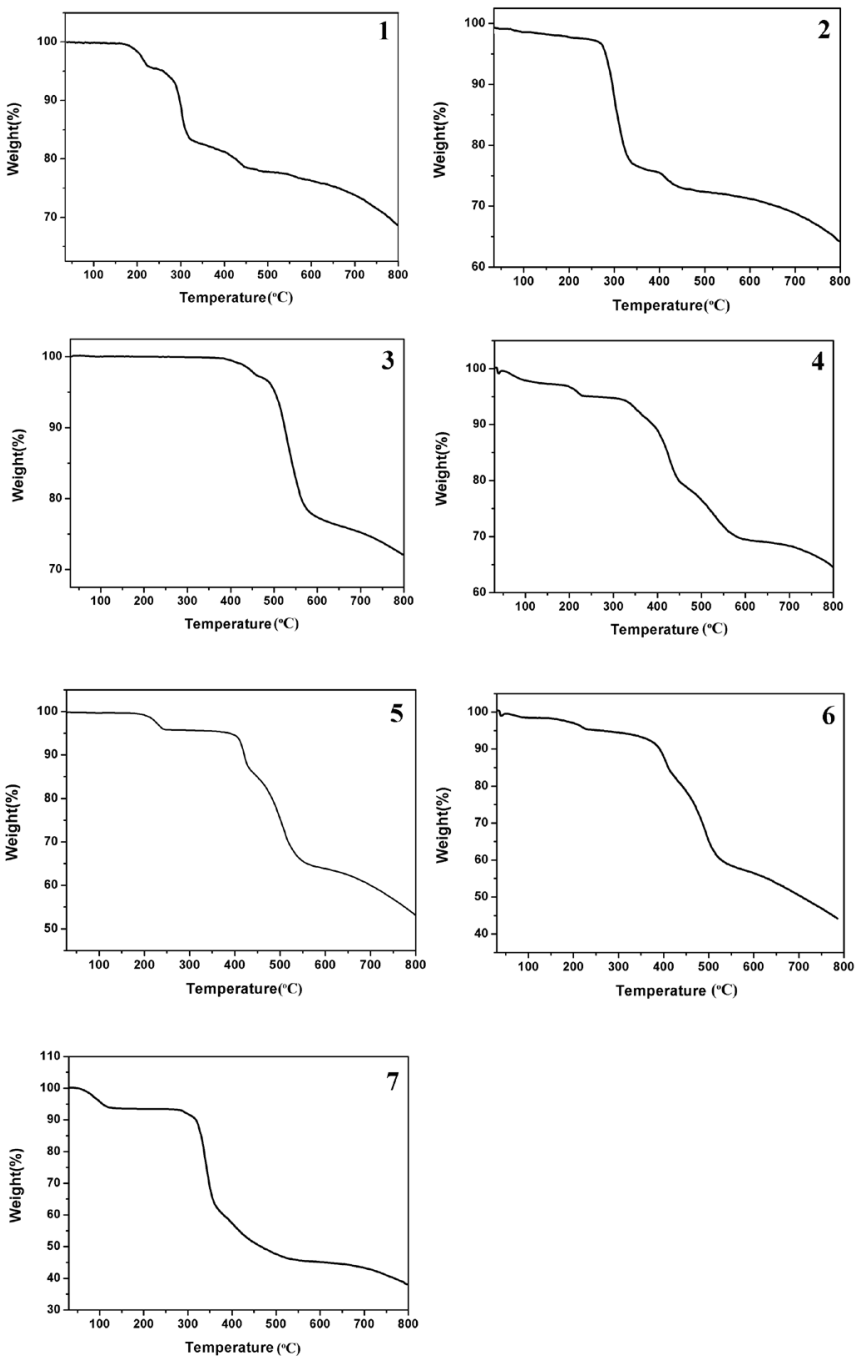

Fig. S3 The TGA curves of compounds **1**-**7**.